Shape Coexistence Around $^{44}_{16}\text{S}_{28}$:

The Deformed N=28 Region

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Abstract

Masses, deformations, radii, and single-particle properties of the very neutron-rich Sulfur isotopes are investigated in the framework of the self-consistent mean-field theory. The stability of the N=28 magic gap around ^{44}S is discussed.

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In contrast to the nuclear structure along the beta-stability line which has been well studied both experimentally and theoretically, the yet unknown structure of drip-line nuclei is currently of great interest [1–3]. From the theoretical point of view, spectroscopy of exotic nuclei offers a unique test of those components of effective interactions that depend on isospin degrees of freedom. Since the parameters of interactions used in the usual mean-field calculations are determined so as to reproduce the properties of beta-stable nuclei, these parameters may not always be optimal around particle drip lines due to (often dramatic) extrapolations involved.

The nuclei discussed in this study are the Sulfur isotopes, especially the neutron-rich ones with N∼28. This particular choice was motivated by recent experimental and astrophysical interest in this mass region [4–6]. From the perspective of the spherical shell model, the underlying proton wave functions are described in terms of the sd shell-model space, while the main neutron components originate from the fp shell-model space. Such a schematic classification, however, easily breaks down due to the strong core polarization effect (i.e., the appearance of static shape deformations associated with the core-breaking excitations). Experimentally, deformed states in magic nuclei are known in many cases (see the recent review [7]). Those *intruders* sometimes appear very low in energy and, in a few cases, they become ground states.

In the sd region, the neutron-rich nuclei with N∼20 are spectacular examples of coexistence between spherical and deformed configurations. A classic example of a magic nucleus with a deformed ground state is $^{32}_{20}$Mg, which has a very low-lying 2^+ state at 886 keV [8] and an anomalously high value of S_{2n}. Calculations based on the deformed mean-field theory predict deformed ground states around ^{32}Mg and explain them in terms of neutron excitations to the $1f_{7/2}$ shell [9,10]. A similar conclusion has been drawn in the shell model calculations in the $(sd)(fp)$ model space [11,12] and in the schematic analysis of ref. [13].

Another region of unexpected collectivity are the $1f_{7/2}$ systems around $^{48}_{24}$Cr$_{24}$. Naively, the main features of these nuclei should be well reproduced in terms of a single-j shell-model picture governed by pairing interaction. However, many properties of the observed states

cannot be accounted for by the results of the empirical $(1f_{7/2})^n$ shell model calculations [14] and the extension to the full (f, p) configuration space is necessary [15,16]. Several nuclei around ^{48}Cr exhibit rotation-like level spacings [17,18] and the self-consistent calculations [19–21] yield deformed ground states. In particular, ^{48}Cr is calculated to be prolate-deformed with quadrupole deformation β_2=0.28 [21].

Experimentally, little is known about the neutron-rich nuclei around ^{44}S. Recently, β-decay properties of ^{44}S and $^{45-47}$Cl have been studied in GANIL [22,4]. The half-life of ^{44}S was found to be $T_{1/2}$=123±10 ms. (Observation of ^{42}Si, ^{45,46}P, ^{48}S, and ^{51}Cl has been reported in ref. [23].) The structure of exotic neutron-rich nuclei with 10<Z<20 will soon be studied at GSI using the fragmentation reaction ^{48}Ca on ^{9}Be at relativistic energies (v/c≈0.5) [5].

Theoretical information on the light N≈28 nuclei is also very scarce. The stability of highly neutron-rich Si isotopes was investigated in ref. [24] in the spherical HF framework with various Skyrme interactions. The results of recent large-scale mass calculations using the finite-range droplet model (FRDM) [25] or the extended Thomas-Fermi with Strutinski-integral model (ETFSI) [26] suggest the presence of deformation in some N=28 isotones (see, e.g., Table IV of ref. [4]). Based on these calculations and on the theoretical analysis of β-decay properties of ^{44}S, it has been suggested in ref. [4] that the influence of the spherical shell N=28 is weakened below ^{48}Ca. The microscopic structure of neutron-rich N∼28 nuclei is important in the astrophysical context. Indeed, the neutron-rich N≈28 nuclei are crucial for the nucleosynthesis of the heavy Ca-Ti-Cr isotopes [4].

To shed some light on the physics of exotic neutron-rich nuclei with N≈28, we performed calculations based on the self-consistent mean-field theory, namely the Skyrme-HF model and the relativistic mean-field (RMF) model. In this Letter we report results for the Sulfur isotopes. The results for the Silicon and Argon isotopes will be published in a forthcoming, more detailed paper.

We perform the Skyrme-HF calculations by discretizing the energy functional on a three-dimensional Cartesian spline collocation lattice, which provides a highly accurate alternative to the finite-difference method [27]. The structure of the resulting lattice representation is

suited for vector and parallel supercomputers, and the method allows for highly modular programming where the order of the splines can be defined as an input parameter. Equations of motion are obtained via the variation of the lattice representations of the constants of motion, such as the total energy. It is worth noting that no self-consistent symmetry has been imposed in the calculations. The details of our method have been published in Ref. [28]. In this work we use the Skyrme interaction SIII [29]. The exchange part of the Coulomb interaction is taken to be in the Slater form. In addition, we use the simple scaling of the nuclear mass to approximately correct for the center-of-mass motion. The calculations were performed in the cube of the size $(20 \text{ fm})^3$. In all the cases considered, the resulting HF minima turned out to correspond to reflection-symmetric shapes with three symmetry planes, i.e., $\langle x \rangle = \langle y \rangle = \langle z \rangle = 0$ and $\langle xy \rangle = \langle xz \rangle = \langle yz \rangle = 0$.

The basic building blocks in the relativistic mean-field approach [30] are the baryons (protons and neutrons) and the $\sigma-$, $\omega-$, and $\rho-$ mesons. The σ-meson is assumed to move in a non-linear potential

$$U(\sigma) = \frac{1}{2}m_\sigma\sigma^2 + \frac{1}{3}g_2\sigma^3 + \frac{1}{4}g_3\sigma^4. \tag{1}$$

In the present work we have employed the recent set of Lagrangian density parameters NL-SH ref. [31]. This set has been claimed to be particularly successful in describing properties of very neutron-rich systems. The relativistic equations of motion are derived by means of the variational principle. The resulting Dirac equation for the baryons and the Klein-Gordon equations for the mesons are solved using the basis expansion method. In this method the small and the large components of the Dirac spinor and the meson fields are expanded in terms of the axially symmetric-stretched harmonic oscillator basis with oscillator frequency $\hbar\omega = 41A^{-1/3}$MeV. (twelve deformed oscillator shells for neutrons and protons were used). In the RMF calculations, only reflection-symmetric axial shapes were considered.

It is known [32] that in drip-line nuclei, pairing interaction leads to the scattering of nucleonic pairs from bound states to continuum. In the mean-field+BCS model this leads to the presence of unphysical "particle gas" surrounding the nucleus. The deficiencies of the

standard treatment of pairing around drip lines can be cured by means of the Hartree-Fock-Bogolyubov (HFB) method with a realistic pairing interaction in which the wave functions of occupied quasiparticle states have correct asymptotic behavior [32]. Unfortunately, the three-dimensional HFB code is not available at present. Consequently, in our study we used the "constant-gap" approximation with a strongly reduced pairing, $\Delta_n = \Delta_p = 75$ keV and 200 keV in the RMF and HF models, respectively. We also performed the RMF calculations with $\Delta_n = \Delta_p = 500$ keV. The results obtained were very similar to those with $\Delta_n = \Delta_p = 75$ keV.

The ground-state minima of the Sulfur isotopes, in most cases, can be associated with deformed intrinsic states. In order to compare various variants of calculations and to relate them to previous work, the standard quadrupole deformation parameters β_2 and γ were extracted. Firstly, the two quadrupole moments, $q_{20} = \sqrt{16\pi/5}\langle r^2 Y_{20}\rangle$ and $q_{22} = \sqrt{8\pi/15}\langle r^2 (Y_{22} + Y_{2-2})\rangle$ were expressed in terms of the polar coordinates $Q_\circ$ and γ [33,34]

$$q_{20} = Q_\circ \cos\gamma, \qquad q_{22} = \frac{1}{\sqrt{3}}Q_\circ \sin\gamma. \tag{2}$$

Using Eq. (2), the γ–value can be determined. The quadrupole moment of proton distribution, $Q_\circ^p$, can be written in terms of β_2^p by means of relation

$$Q_\circ^p = \sqrt{\frac{5}{\pi}}Z\langle r_p^2\rangle\beta_2^p. \tag{3}$$

Similarly, one can extract quadrupole deformations of neutron (β_2^n) and mass (β_2^A) distributions. Since, in most cases, the equilibrium shapes predicted by the HF model are axial, we adopted the standard convention (i.e., $\beta_2 > 0$ (prolate) for $\gamma \sim 0°$ and $\beta_2 < 0$ (oblate) for $\gamma \sim 60°$).

The two-neutron separation energies for the Sulfur isotopes, S_{2n}, are displayed in Fig. 1 as a function of neutron number. Our HF and RMF results are compared with the predictions of the FRDM and ETFSI models, and experimental data. In general, the agreement between the models themselves and between theory and experiment is good. In the HF

model the nucleus ^{52}S (N=36) is two-neutron-unstable. The RMF calculations yield more neutron binding; the isotopes ^{52,54}S are predicted to lie inside the two-neutron drip-line. The systematic model agreement for S_{2n} should not imply that the intrinsic structures of neutron-rich Sulfur isotopes are also similar in all models presented in Fig. 1. As discussed below, this is not the case.

The calculated mass quadrupole deformations of even-even Sulfur isotopes are shown in Fig. 2 as a function of neutron number. (Usually, calculations yield more than one energy minimum. In such situations, deformations and excitation energies of excited states are also displayed.) The deformation pattern for even-even isotopes $^{28-38}$S is fairly similar in the HF and RMF models: prolate ground states in $^{28-32,38}$S, oblate minimum in ^{34}S, and spherical shape in the magic N=20 nucleus ^{36}S‡. However, the differences show up for the heavier isotopes.

The nuclei ^{40,42}S are predicted by the RMF model to have prolate ground states with $\beta_2 \sim 0.25$; the oblate minima with $\beta_2 \sim$-0.16 lie about 4 MeV higher in energy. In the HF calculations, prolate ($\beta_2 \sim 0.25$) and oblate ($\beta_2 \sim$-0.24) configurations are practically degenerate. The FRDM and ETFSI models give prolate-deformed ground states with ($\beta_2 \sim 0.25$), in agreement with our findings.

There is no consensus regarding the equilibrium shape of the N=28 nucleus ^{44}S. According to RMF calculations, ^{44}S has a well-deformed prolate ground state with β_2=0.31. The oblate minimum with β_2=0.16 appears to lie 0.8 MeV higher. The spherical saddle point lies even higher at E^*=2.8 MeV. On the other hand, according to the HF model, ^{44}S is a gamma-soft system with a small quadrupole deformation $\beta_2 \sim 0.13$. The very shallow, well-deformed prolate minimum (β_2=0.28) analogous to the RMF ground state lies at $E^* \sim 1.5$ MeV. The

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‡It is to be noted here that RMF predicts a slightly deformed shape for ^{36}S. This can be attributed to very weak pairing in the calculations. If a stronger proton pairing gap is assumed, Δ_p=1 MeV, the equilibrium shape becomes spherical.

FRDM and ETFSI models give spherical and oblate (β_2=–0.26) ground states, respectively.

The heavier Sulfur isotopes with N>28 are consistently calculated to be prolate-deformed in the HF, RMF, and FRDM models. The oblate minima are higher in energy, but with increasing neutron number, the prolate-oblate energy difference is reduced. The RMF approach yields systematically larger quadrupole deformations compared to HF. For instance, according to the RMF predictions, ^{48}S is a well-deformed system with β_2=0.22. According to the HF model, it is a transitional nucleus with β_2=0.13, γ=10°. Interestingly, the ETFSI approach favors a strongly deformed oblate configuration with β_2=–0.25.

For the N=28 isotone, ^{42}Si calculations yield well-deformed oblate ground states with β_2 ranging from –0.32 (FRDM) to –0.22 (HF). Also, for the Silicon isotopes, the RMF model gives slightly more neutron binding than HF. According to RMF, the nucleus ^{48}Si is still inside the two-neutron drip-line, while it is unstable in the HF model. Another N=28 isotone, ^{46}Ar, is predicted to be spherical (RMF, FRDM) or oblate (HF) with β_2=–0.14. The RMF model gives an oblate minimum with β_2=–0.10 at very low excitation energy. This indicates the transitional character of ^{46}Ar.

Figure 3 displays the representative single-particle neutron levels as functions of quadrupole deformation β_2. The Nilsson diagram was obtained using a deformed Woods-Saxon model with a Chepurnov set of parameters [35]; the resulting single-particle energies are close to those from the HF+SIII model. (In the RMF–NL-SH calculations the order of $s_{1/2}$ and $d_{3/2}$ shells is reversed.) The neutron and proton single-particle levels in the ground-state of ^{44}S obtained in HF and RMF models are also displayed in Fig. 3. The deformed shape in ^{44}S results from a subtle interplay between the deformed gaps at Z=16 and N=28, and the spherical N=28 gap. In the RMF model, the spherical N=28 gap is completely broken; the neutron intruder orbital [321]1/2, originating from the $2p_{3/2,1/2}, 1f_{5/2}$ shells above the N=28 gap is occupied. In the HF calculations the energy distance between the deformed [321]1/2 and [303]7/2 levels is only 1.6 MeV.

The predicted root-mean-square (rms) neutron and charge radii of even-even Sulfur isotopes are illustrated in Fig. 4. The results of HF and RMF models are fairly similar. There

appears a systematic shift of ~ 0.08 fm between the HF and RMF results for the rms charge radii; the experimental data for ^{32,34,36}S lie in between. As expected, due to skin effect, rms radii increase when approaching particle drip-lines. (Since, in our study, the pairing correlations are practically neglected, the undesired "particle gas" effect mentioned above is not present.)

The difference between neutron and proton deformations, $\Delta\beta_2 \equiv \beta_2^n - \beta_2^p$, is illustrated in Fig. 5. It is seen that when approaching the neutron drip-line, the values of β_2^n are systematically smaller than those of the proton distribution. An opposite effect is seen around the proton drip-line. The largest difference, $|\Delta\beta_2| \sim 0.10$, is obtained in the RMF model for ^{54}S. (As discussed above, the deviation for ^{36}S disappears if the stronger proton pairing gap is assumed.) The behavior of $\Delta\beta_2$ can be partly attributed to the isotonic behavior of rms radii in Fig. 4 (see the definition (3) of β_2). Indeed, the value of $Q_\circ$ depends both on the angular anisotropy *and* the radial dependence of the nucleonic density. In the drip line nuclei, due to spatially extended wave functions, the "radial" contribution to $Q_\circ$ might be as important as the "angular" part. Moreover, it can strongly depend on particle number. The insert in Fig. 5 illustrates the dependence of the $Q_\circ^n/Q_\circ^p$ ratio on the N/Z ratio. Up to neutron number N=26 the HF and RMF results are very similar. The dips in $Q_\circ^n/Q_\circ^p$ in the HF calculations appear at shell and subshell closures (i.e., at N=14, 20, 28, and 32). At these particle numbers the neutron distribution has a tendency to be more spherical. The lack of shell fluctuations in $Q_\circ^n/Q_\circ^p$ in the RMF model at N>26 is consistent with the calculated large prolate deformations. Interestingly, above N=28, $\Delta\beta_2$(RMF) decreases steadily with neutron number, while the $Q_\circ^n/Q_\circ^p$(RMF) ratio intersects the N/Z line (rigid geometric limit) only at N>34.

In summary, our calculations suggest strong deformation effects in the region around ^{44}S due to the $1f_{7/2} \rightarrow fp$ core breaking. Large differences between neutron and proton quadrupole moments are obtained in the RMF approach in deformed Sulfur nuclei far from stability. Such differences might have interesting consequences for the quadrupole isovector modes in drip line systems. According to the RMF+NL-SH model, the N=28 nuclei ^{44}S

and ^{42}Si are well deformed in their ground states. On the other hand, the HF+SIII model predicts smaller deformations, and ^{44}S is calculated to be a soft transitional system. The new experimental data around ^{44}S will certainly be very helpful in pinning down the question of quadrupole collectivity in this mass region.

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FIGURES

FIG. 1. Two-neutron separation energies of the even-even Sulfur isotopes calculated with the HF and RMF models. They are compared with the results of the FRDM [25] and ETFSI [26] models, and experimental data.

FIG. 2. Quadrupole mass deformations β_2^A of the even-even Sulfur isotopes calculated with the HF (top) and RMF (bottom) models. The dots connected by a solid line correspond to ground-state deformations. The empty circles indicate excited configurations (with excitation energies given in MeV).

FIG. 3. Left: Woods-Saxon single-particle neutron levels as functions of β_2. The orbitals are labeled by means of Ω and π (π=+, solid line; π=−, dashed line) quantum numbers. Right: The shell structure of ^{44}S as predicted by the HF and RMF models.

FIG. 4. Root-mean-square radii of the neutron distribution (top) and charge distribution (bottom) of the even-even Sulfur isotopes calculated with the HF and RMF models. The radii are shown relative to the average (liquid-drop) value of $\sqrt{3/5}R_\circ$, $R_\circ = 1.2A^{1/3}$ fm. The experimental data for ^{32,34,36}S are taken from ref. [36]

FIG. 5. Difference $\Delta\beta_2 \equiv \beta_2^n - \beta_2^p$ for the even-even Sulfur isotopes calculated with the HF and RMF models as a function of neutron number. The insert shows the ratio of neutron and proton quadrupole moments versus N/Z. The large-deformation excited state in ^{44}S calculated in the HF model is indicated by means of an "($\bullet$)" symbol.

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